

Research papers

Generation of root zone soil moisture from the integration of an all-weather satellite surface soil moisture estimates and an analytical model: A preliminary result in China

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ABSTRACT

In addition to surface soil moisture (SSM) data, root zone soil moisture (RZSM) is particularly significant for irrigation decision-making and agricultural drought warnings since water uptake generally occurs through the root systems of plants. In this study, a daily/0.05° RZSM dataset covering the major land areas of China was generated from the synergistic use of satellite-derived SSM estimates and a RZSM-SSM analytical model. First, based on the SSM and RZSM datasets generated from the fifth generation of atmospheric reanalysis (ERA5-Land), the Markov Chain Monte Carlo algorithm was applied to optimize the soil moisture analytical relationship (SMAR) model to determine four essential parameters pixel-to-pixel over the study area. In addition, the optimized SMAR parameters were integrated with satellite-derived daily/0.05° SSM to predict the daily/0.05° RZSM in China. Finally, due to the lack of in situ RZSM measurements ground truth at a spatial resolution of 0.05°, two RZSM products, namely the Soil Moisture Active Passive (SMAP)-based RZSM and the China Meteorological Administration Land Data Assimilation System (CLDAS)-based RZSM, were used as references to preliminarily assess the estimated data. The results showed overall fair correlations between SMAP RZSM and estimated RZSM (correlation coefficient R varying from 0.557 to 0.655), and between CLDAS RZSM and estimated RZSM (correlation coefficient R varying from 0.496 to 0.596) over four typical days representing spring, summer, autumn, and winter in 2019. Although the proposed approach may overestimate or underestimate RZSM compared to the two referenced products in different seasons, an overall acceptable accuracy with unbiased root mean square error of $\sim 0.070\text{--}0.090\text{ cm}^3/\text{cm}^3$ was obtained.

1. Introduction

As a crucial component of the soil moisture (SM) profile, root zone soil moisture (RZSM) plays an important role in various fields, such as agriculture, hydrology, and meteorology (Choi et al., 2021; Gheybi et al., 2019; Sure and Dikshit, 2019; Zhuang et al., 2020). Specifically, it is widely recognized that RZSM is a controlling factor in these

applications, whereas most of the currently available satellite-based methods only focus on the SM of the top soil layer (e.g., surface soil moisture, SSM) (Dumedah et al., 2015). Taking agricultural irrigation and water consumption as an example, irrigation water or precipitation from the atmosphere infiltrates the root zone soil layer via the upper soil; hence, only water that reaches the crop root can be absorbed by root systems; then, the absorbed water returns to the atmosphere by

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vegetation transpiration. This entire water cycle in the soil–vegetation–atmosphere system is not only the basic requirement of vegetation physiological processes but also the main path by which nutrients are delivered to maintain the ecological functions of crops. Therefore, the monitoring of RZSM is critical for crop growth monitoring, yield prediction, field irrigation decision-making and early agricultural warning (Choi et al., 2021; Grillakis et al., 2021; Pablos et al., 2018; Xu et al., 2021).

Currently, satellite-based RZSM estimation can be broadly divided into two categories. One is a direct method by which RZSM is obtained with low-frequency active microwaves (e.g., P-band radar), whose signals can successfully penetrate deep soil layers (Etminan et al., 2020; Garrison et al., 2017; Sadeghi et al., 2017; Yueh et al., 2020). However, such investigations are still in their early stages, and only a few satellite missions are scheduled to carry P-band radar (for example, both NASA's SNoPI and ESA's Biomass are expected to be launched in 2024) (Etminan et al., 2020; Sadeghi et al., 2017; Tabatabaenejad et al., 2015, 2020). In addition, several studies have highlighted the feasibility of estimating RZSM from visible/near-infrared (VIS/NIR) or thermal infrared (TIR) observations, as VIS/NIR or TIR-based evapotranspiration or transpiration have the capacity for inferring water conditions within the root layer (Alburn et al., 2015; Akuraju et al., 2021; Scott et al., 2003; Pradhan 2019; Pradhan et al., 2020). However, it is widely recognized that VIS/NIR or TIR measurements are easily contaminated by clouds (Metz et al., 2017; Li et al., 2018; Pham et al., 2019), making it difficult to obtain spatially complete RZSM. Moreover, most of the currently available relationships between RZSM and satellite evapotranspiration or transpiration measurements are still empirical ones that depend on local atmosphere, soil, and vegetation conditions (Akuraju et al., 2021; Holzman et al., 2021).

The other method indirectly estimates RZSM by assimilating SSM into a hydrological or land surface model (Martens et al., 2017; Tian et al., 2019). Currently, most mainstream microwave-based SSM products, such as the Soil Moisture Active Passive (SMAP) and the Soil Moisture and Oceanic Salinity (SMOS), have been used to generate RZSM products through assimilation processes (Pablos et al., 2018; Reichle et al., 2019; Xing et al., 2021). Compared to the direct method for obtaining RZSM, assimilation-based methods have received more attention. However, most of the currently available assimilated RZSM products are characterized by the spatial resolution of tens of kilometers. For instance, the widely used Global Land Data Assimilation System and the North American Land Data Assimilation System operate at the spatial resolution of 25 km and 12.5 km, respectively. Despite the global high-resolution capability of the land information system (LIS) due to significant hardware and software improvements, there are currently no operational RZSM products at a national scale with a relatively high spatial resolution (e.g., 1–5 km) to the best of our knowledge. Nevertheless, achieving this goal in future developments is anticipated, as computational challenges of high-resolution land surface modeling have been effectively addressed (Kumar et al., 2006; 2008a, Kumar et al., 2008b). It is well known that the LIS typically requires a large number of observations to routinely produce RZSM and other output through the assimilation system and the mechanism of assimilation is to optimize the target variables, which may result in poor physical interpretation of other parameters (Fiedler et al., 2022; Houtekamer and Zhang, 2016). Although there are limitations to the assimilation systems from a computational and data requirements perspective, it is noteworthy that they are capable of providing useful inputs for various land surface process studies including model parameters optimization and land surface variables estimation (Li et al., 2024). Another drawback is that it is difficult for the land surface or hydrological model to reflect human activities timely. For example, when an irrigation event occurs, the farmland gets wetter, and this change can be easily detected by either TIR or microwave sensors, but not by land surface or hydrology model in time. This is one of the most significant advantages of remote sensing technology.

In recent years, analytical models have been widely used to obtain RZSM. A typical model is the soil moisture analytical relationship (SMAR) model developed by Manfreda et al. (2014). The main idea of the SMAR model is to divide the soil column into two sections, the surface layer and root layer, and the vertical movement of liquid water from the surface layer to the root layer follows the Green-Ampt infiltration equation. Specifically, the development of the SMAR generally follows a previous work by Wagner et al. (1999), who used the exponential filtering method with an attenuation constant to characterize the dynamic change in RZSM using time-series SSM observations, which has been extensively applied to improve the description of RZSM in the "precipitation-runoff" model (Brocca et al., 2010, 2012; Manfreda et al., 2014; Matgen et al., 2012). Following the SMAR model, many scholars have investigated RZSM estimation at various spatial scales. Gheybi et al. (2019) implemented the SMAP-derived SSM product into the SMAR model to monitor RZSM at five stations in Iran, providing an average root mean square error (RMSE) of $0.058 \text{ cm}^3/\text{cm}^3$. Farokhi et al. (2021) integrated downscaled microwave-based SSM data into the SMAR model, showing that the performance of SMAR increased when using downscaled SSM compared to the original resolution SSM. Furthermore, Baldwin et al. (2019) first attempted to obtain regional RZSM at a 1 km spatial resolution with the SMAR model over the eastern United States region. In their study, the SMAR parameters at 1 km spatial resolution over the study area were determined from the integration of site calibration and neural network-based upscaling technology. However, it is widely recognized that neural network-based algorithms commonly require plenty of training data, which may not be suitable for regions with relatively sparse measurements.

In recent years, many methods have been developed to remove the effects of clouds and restore ground information for satellite images (Lv et al., 2018; Song et al., 2021; Zhou et al., 2022), providing an unprecedented opportunity to obtain spatially and temporally continuous SSM estimates at relatively fine resolution ($\sim 1 \text{ km}$) (Myer et al., 2022; Toride et al., 2019; Zhang et al., 2023). Specifically, these seamless fine-resolution- satellite-derived SSM datasets can serve as the unique input for the SMAR model to predict RZSM. Meanwhile, to predict RZSM with the SMAR model over a large area, except for the integration of site measurements and neural network-based upscaling, the release of the fifth generation of atmospheric reanalysis (ERA5-Land) with a resolution of 0.1° also provides an alternative for the optimization of the analytical model pixel-to-pixel in regional scale. The primary motivation for the present study is to develop a practical framework for generating high spatial resolution RZSM (e.g., 0.05° that is approximately centered between the $\sim 1 \text{ km}$ satellite SSM estimates and 0.1° reanalysis data of ERA5-Land) from the integration of satellite-derived SSM data and the SMAR model over the vast country of China. The main advantage of the present study is to explore the feasibility of optimizing the SMAR model with reanalysis data since previous studies generally used site-based measurements, which are difficult to apply over large regions or data-scarce areas. In addition, compared to other approaches (e.g., land surface modeling/assimilation, machine/deep learning) for obtaining root zone soil moisture dataset, the proposed method is a more direct and simple way because only satellite-derived SSM is required as input. After the introduction, the paper is organized as follows: Section 2 explains the methods, Section 3 describes the study area and data, Sections 4 and 5 present the results and discussion, respectively, and Section 6 summarizes the study.

2. Methods

The methodology adopted in the present paper is described in the flow chart (Fig. 1), which is divided into three steps: (i) optimization of SMAR parameters; (ii) estimation of SSM; and (iii) assessments of SSM/RZSM. The following subsections illustrate the three steps in detail.

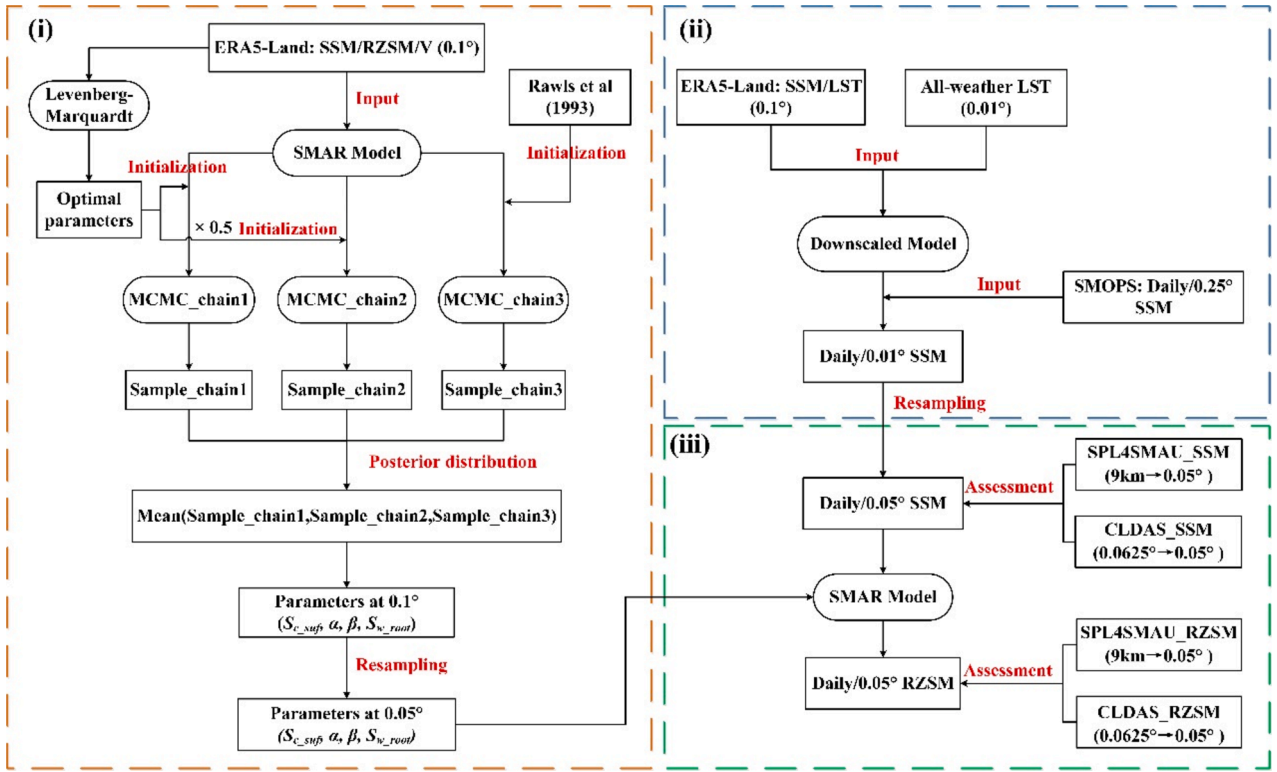


Fig. 1. Flow chart of the present study. The entire approach for the generation of the daily/0.05° RZSM includes three steps: (i) optimization processes for the determination of the SMAR parameters; (ii) estimation of SSM to be used as input of the SMAR model; (iii) assessments of the estimated SSM and RZSM with referenced data.

2.1. Optimization of SMAR parameters

2.1.1. Brief description of the SMAR model

The SMAR model was first proposed by Manfreda et al. (2014), where water in the surface layer (i.e., satellite-derived SSM) is assumed to infiltrate into the root layer (i.e., RZSM) when it exceeds the relative saturation at the field capacity. In recent years, SMAR models have been widely used to obtain RZSM at various scales (Baldwin et al., 2019; Faridani et al., 2017; Farokhi et al., 2021; Gheybi et al., 2019; Guo et al., 2023; Zhuang et al., 2020). This section provides only a brief introduction to the SMAR model, more details on the physical mechanism and major assumptions of the SMAR model can refer to Manfreda et al. (2014). In the SMAR model, a parameter of S_{c_surf} is used to decide whether infiltration occurs from the surface to the root layer. Specifically, S_{c_surf} is defined as the relative saturation at the field capacity for the surface layer.

Following the principle of soil water balance, the SMAR model for the root layer can be written as follows:

$$(1 - S_{w_root})P_{root}D_{root}\frac{dx_{root}(t)}{dt} = P_{surf}D_{surf}y(t) - V_{root}x_{root}(t) \quad (1)$$

where P_{surf} and D_{surf} are the soil porosity and soil depth for the surface layer; P_{root} , D_{root} , and S_{w_root} are the soil porosity, soil depth, and the relative saturation at the wilting point for the root layer, respectively; V_{root} is the soil water loss coefficient due to evapotranspiration and percolation losses; $x_{root}(t)$ is the effective relative soil saturation in the root layer at time t ; $y(t)$ represents the fraction of soil saturation permeating into the root layer at time t .

Equation (1) can be transformed to integral form as follows:

$$\int \frac{dx_{root}(t)}{dt} = \frac{P_{surf}D_{surf}}{(1 - S_{w_root})P_{root}D_{root}} \times \int y(t) - \frac{V_{root}}{(1 - S_{w_root})P_{root}D_{root}} \times \int x_{root}(t) \quad (2)$$

To simplify the expression in equation (2), we use α and β to represent the constant items $\frac{V_{root}}{(1 - S_{w_root})P_{root}D_{root}}$ and $\frac{P_{surf}D_{surf}}{(1 - S_{w_root})P_{root}D_{root}}$, respectively. Specifically, α can represent normalized daily root zone water loss whereas β can control the diffusion rate of excess water into the root zone. Then, equation (2) can be written as follows:

$$\int \frac{dx_{root}(t)}{dt} = \beta \times \int y(t) - \alpha \times \int x_{root}(t) \quad (3)$$

Manfreda et al. (2014) assumed an initial condition for the relative saturation $x_{root}(t)$ equal to zero, and one may derive an analytical solution as follows:

$$x_{root}(t) = \int_0^t \beta e^{\alpha(\omega-t)} y(\omega) d\omega \quad (4)$$

By converting the integral form to the discrete form, one can yield:

$$x_{root}(t_j) = \sum_{i=0}^j \beta e^{\alpha(t_i-t_j)} y(t_i) \Delta t \quad (5)$$

To better calculate RZSM from a time series of SSM measurements for a given location, it is assumed that $\Delta t = t_j - t_{j-1}$, and RZSM at time t can be written as a temporally discrete form as follows:

$$S_{root}(t_j) = S_{w_root} + [S_{root}(t_{j-1}) - S_{w_root}] e^{-\alpha \Delta t} + \beta y(t_j) \Delta t (1 - S_{w_root}) \quad (6)$$

where $S_{root}(t)$ is the relative RZSM at the time t .

2.1.2. Optimization processes

Based on the equations above, the SMAR model requires the calibration or estimation of four parameters (S_{c_surf} , S_{w_root} , α , β) to describe the relationship between RZSM and SSM. Specifically, Bayesian inference deduces the posterior state about a set of parameters as the result of prior information about a set of parameters and likelihood function. In the present study, the Markov Chain Monte Carlo (MCMC) algorithm was selected for the Bayesian inference to optimize the SMAR model to obtain the four parameters (S_{c_surf} , S_{w_root} , α , β) pixel-to-pixel over the study area. Currently, MCMC is an increasingly useful method for obtaining distribution information, especially for estimating posterior distributions in Bayesian inference because the focus on posterior distributions is often difficult to solve with the analytical examination. Consequently, MCMC allows users to approach aspects of posterior distributions that cannot be directly calculated (e.g., random samples from the posterior) (Don et al., 2018). The power of the MCMC algorithm is not only beneficial for Bayesian inference, but it also has been widely employed in other domains, such as statistics, psychology, and other vast range of research paradigms (Don et al., 2018; Gallant et al., 2022; Yang and Bao, 2019; Ma et al., 2017; Ma et al., 2022).

The parameter optimization was conducted using modMCMC, a function in the R FME package that implements the MCMC algorithm with delayed rejection and adaptive Metropolis procedures (Haario et al., 2006; Soetaert and Petzoldt, 2010). Specifically, the MCMC algorithm requires at least two years of SSM, RZSM and soil water loss measurements as prior knowledge for optimizing the four parameters (S_{c_surf} , S_{w_root} , α , β). The SSM/RZSM should be converted to relative quantities (S_{c_surf}/S_{w_root}) using the soil porosity with different soil textures shown in Table 1 according to Rawls et al. (1993). If S_{c_surf} and S_{w_root} are greater than one, the corresponding soil porosity should be appropriately adjusted to ensure that more than 95 % of S_{c_surf} and S_{w_root} are between 0 and 1.

As shown in Fig. 1, three MCMC chains with various initial values and iteration periods were determined, where the minimum negative log-likelihood was set as the objective function. To run the MCMC chain, an initial set of the four SMAR parameters (S_{c_surf} , S_{w_root} , α , β) were obtained by operating the Levenberg-Marquardt derivative algorithm and were subsequently used as the input for the first MCMC chain, where the iterations were set as 9000 for each pixel, including 3000 iterations as the burn-in period; for the second MCMC chain, the initial values were set to half of the first chain, with 18,000 iterations and a burn-in period of 12,000 iterations; for the third chain, the initial value was set to the model parameters corresponding to different soil textures derived from the experimental investigations by Rawls et al. (1993), which are shown in Table 1. Specifically, to guarantee that the output iterations in the three MCMC chains were the same, the iterations and burn-in period of the third MCMC chain were set to be the same as those of the first. In addition, following the built-in pattern in the SMAR model, all the parameters in the SMAR model were used as “relative dimension” terms, rather than the actual physical variables. Hence, the lower and upper bounds of each parameter were set to 0 and 1, respectively.

Table 1

The soil parameters associated with different soil textures for the SMAR model.

Soil type	P (soil porosity)	S_{c_surf}	S_{w_root}
Sand	0.437	0.14	0.06
Loamy sand	0.437	0.24	0.11
Sandy loam	0.453	0.42	0.19
Silty loam	0.501	0.57	0.27
Loam	0.463	0.50	0.25
Sandy clay loam	0.398	0.62	0.34
Silty clay loam	0.471	0.73	0.45
Clay loam	0.464	0.67	0.40
Sandy clay	0.430	0.75	0.51
Silty clay	0.479	0.78	0.52
Clay	0.475	0.80	0.56

As a result of the considerably distributed initial values in the three chains, SMAR parameters may be broadly sampled within the possible value range (Baldwin et al., 2019). After transforming the stable distributions of the three chains into the posterior distribution of parameters for estimations, the Gelman-Rubin test was used to determine if they converged to the same stationary parameter space; the mean of the posterior parameter distributions of the three MCMC chains was then taken as the final parameter estimation. Finally, the RMSE and the correlation coefficient (R) were adopted to evaluate the quality of model parameter optimization.

2.2. Estimation of SSM

Following the description of the SMAR model, SSM is an essential input for generating RZSM using the proposed approach. To estimate the all-weather daily/0.05° RZSM dataset, it is quite necessary to obtain spatially and temporally continuous SSM estimates in advance with the proposed framework. In the present study, the method proposed by Zhang et al. (2023) was primarily used to generate daily/1-km SSM with quasi-full spatial coverage. The method can be generally divided into three steps: the first step is to develop relationships between SSM and day/night land surface temperature (LST) difference over groups of land cover types and vegetation levels at a relatively coarse spatial scale; then, the relationships are applied to fine resolution day/night LST satellite products to obtain an initial SSM dataset; at last, microwave-based SSM products are used to correct the initial SSM for the obtaining of the final SSM datasets. A preliminary assessment of the estimated SSM generally revealed comparable or better accuracy than other microwave-based SSM products (Zhang et al., 2023). More detailed information on this method can be found in Zhang et al. (2023) and Fang et al. (2022). Based on Zhang et al. (2023), daily/1-km SSM was first obtained and further aggregated to a spatial resolution of 0.05° in further investigation.

2.3. Assessments of SSM/RZSM

In the present study, because it is quite difficult to obtain ground SSM and RZSM truth at a spatial resolution of 0.05° over the study region, a satellite-based and a land data assimilation system-based SSM/RZSM products were initially resampled to the spatial resolution of 0.05° and subsequently taken as references to preliminarily evaluate the estimated SSM and RZSM datasets. Specifically, four statistical criteria, including RMSE, bias, unbiased RMSE (ubRMSE) and R , were used in the present study to quantitatively assess the accuracy of the estimated SSM and RZSM against reference datasets. The statistical criteria are written as follows:

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (Y_i - X_i)^2}{n}} \quad (7)$$

$$Bias = \frac{\sum_{i=1}^n (Y_i - X_i)}{n} \quad (8)$$

$$ubRMSE = \sqrt{RMSE^2 - Bias^2} \quad (9)$$

$$R = \frac{\sum_{i=1}^n (X_i - \bar{X})(Y_i - \bar{Y})}{\sqrt{\sum_{i=1}^n (X_i - \bar{X})^2} \sqrt{\sum_{i=1}^n (Y_i - \bar{Y})^2}} \quad (10)$$

where n is the number of sampling pixels; X_i and Y_i are the referenced SSM (or RZSM) products and estimated SSM (or RZSM) datasets, respectively; and $\bar{X}$ and $\bar{Y}$ are the averages of the corresponding data.

3. Study region and data

3.1. Study region

In the present study, the entire land area of China (including two major islands of Hainan and Taiwan) was taken as the study region to generate the daily/0.05° RZSM product. The study region is located in eastern Asia and the west coast of the Pacific Ocean, between 18.1° N–53.6° N latitude and 73.3° E–135.1° E longitude. As the largest agricultural and developing country, China is expected to feed over 1.4 billion people with limited [cultivated land](#). It is of great significance to investigate the spatiotemporal distribution and dynamics of RZSM in China due to the critical role of RZSM in agricultural developments, especially in a water-scarcity country such as China. The [vast territory](#) of the study region contains diverse landscapes and climate patterns. [Fig. 2](#) depicts the major land cover types based on the Moderate-Resolution Imaging Spectroradiometer (MODIS) product (MCD12Q1C).

3.2. Data description

[Table 2](#) shows the primary data used in the present investigation. The following subsections provide a thorough description of these data.

3.2.1. ERA5-Land reanalysis data

Developed by the European Center for Medium-Range Weather Forecasts (ECMWF), ERA5-Land is the fifth generation of atmospheric reanalysis of global climate with a high spatiotemporal resolution of 0.1°/hourly. Currently, ECMWF can provide a consistent view of the evolution of land variables from 1950 to the present, and the monthly aggregates of the hourly products can also be obtained ([Muñoz-Sabater et al., 2021](#)). It is noteworthy that a large number of historical observations have been considered in the modelling and assimilation systems for producing the ERA5-Land reanalysis. Specifically, the number of observations assimilated in the ERA5-Land systems has increased from approximately 0.75 million per day on average in 1979 to around 21 million per day by July 2018. Hence, the ERA5-Land has been recognized to be a more accurate reanalysis and a better real-time forecast. In the ERA5-Land framework, SM is divided into four layers with varying depths (layer 1: 0–7 cm, layer 2: 7–28 cm, layer 3: 28–100 cm, and layer 4: 100–289 cm). In the present study, the first layer with a depth of 7 cm

Table 2

Description of primary data required in this study.

Dataset	Variable	Spatial resolution	Time range	Function
ERA5-Land	SSM/RZSM V(Runoff/Total evaporation)	0.1°	2014–2017	Optimization of SMAR parameters (Baldwin et al., 2019)
ERA5-Land	SSM/LST	0.1°	2019	SSM estimation (Zhang et al., 2023)
SMOPS	SSM	0.25°	2019	
TRIMS	LST	0.01°	2019	
LST				
SMAP	SSM	0.09°	2019	Assessments of SSM
	RZSM	0.09°	2019	Assessments of RZSM
CLDAS	SSM	0.0625°	2019	Assessments of SSM
	RZSM	0.0625°	2019	Assessments of RZSM

was considered as the surface layer, and SM within this layer was recognized as SSM. Moreover, the second and third layers were set as the root layer, and the averaged SM in the two layers was used as RZSM. Hence, the optimized SMAR parameters and estimated RZSM generally refer to the depth from 7 to 100 cm. Apart from SM, several other ERA5-Land variables, such as total evaporation, runoff, and LST, were also used to investigate RZSM estimation in the present study. All these data can be obtained from the Climate Data Store website (<https://cds.climate.copernicus.eu/>).

3.2.2. SMOPS SSM and TRIMS LST products

In addition to the four SMAR parameters (S_{c_surf} , S_{w_root} , α , β), SSM is required to generate RZSM in the SMAR model as described in [Fig. 1](#). In the present study, daily/1-km SSM was obtained from the synergetic use of reanalysis data and satellite products of all-weather LST and SSM, following the method proposed by [Zhang et al. \(2023\)](#). Furthermore, the daily/1-km SSM was aggregated to a spatial resolution of 0.05° to estimate the final RZSM. Specifically, this resolution of 0.05° is reasonable because it is generally an intermediate scale between the original resolution of the SSM (0.01°) and the SMAR parameters (0.1°) optimized

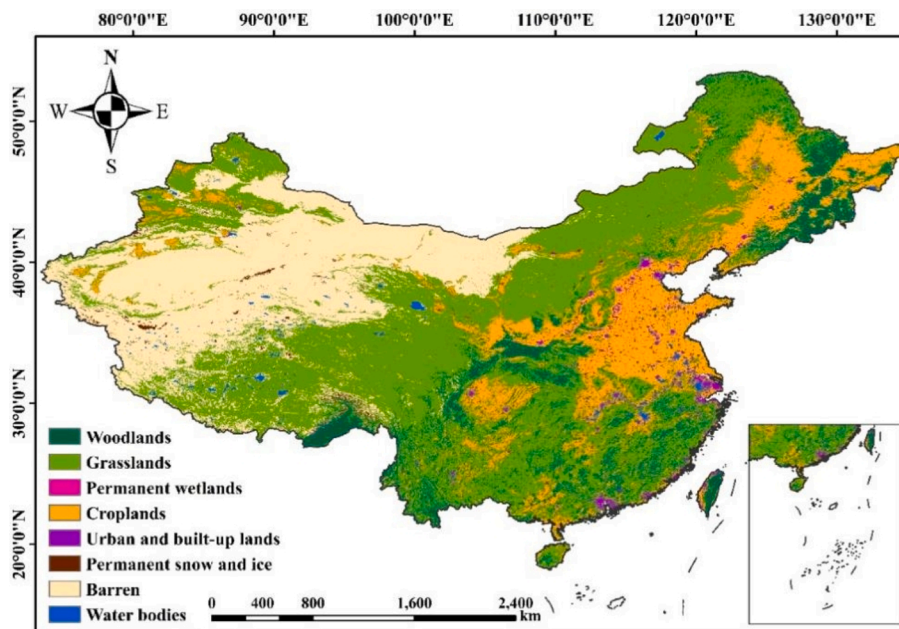


Fig. 2. Land cover types of the study region based on the MCD12Q1C product.

based on the ERA5-Land data.

To this end, the daily Soil Moisture Operational Product System (SMOPS) with a spatial resolution of 0.25° was introduced for further investigation. SMOPS has combined SSM retrievals from multiple satellite sensors to make use of all available microwave-based data; it has been managed by the National Oceanic and Atmospheric Administration (NOAA) since 2012. The main reason for the selection of the SMOPS product is due to its quasi-full spatial coverage, which is superior to other microwave-based SSM products (Yin et al., 2020). In the present study, the latest version of SMOPS (v3.0) with enhanced accuracy was used as the satellite SSM product to generate the daily/ 0.05° SSM. The SMOPS product was obtained from the NOAA website (<https://www.ospo.noaa.gov/Products/land/SMOPS/>).

In addition to SMOPS SSM, another satellite data used for the generation of daily/ 0.05° spatially complete SSM is the all-weather Thermal and Reanalysis Integrating Moderate-resolution Spatial-seamless (TRIMS) LST product. Specifically, the TRIMS LST product was derived from the synergistic use of MODIS and Global Land Data Assimilation System-derived LST as well as auxiliary data on vegetation index and land surface albedo according to the algorithm developed by Zhang et al. (2021). Compared to traditional thermal-based LST products, all-weather TRIMS LST can fill the gaps left by cloud contaminations. Recent assessments of the TRIMS LST product against 15 sites in China showed a better accuracy (overall RMSE of 1.52–3.71 K) than other all-weather LST products (Zhang et al., 2019, 2021; Zhou et al., 2017). The TRIMS LST product was obtained from the National Qinghai-Tibet Plateau Scientific Data Center (<https://data.tpdc.ac.cn/en/data>).

3.2.3. SMAP products

In the present study, due to the lack of ground-based SSM/RZSM at a spatial resolution of 0.05° over the study region, the SMAP product resampled to 0.05° was taken as a reference to preliminarily evaluate the estimated SSM/RZSM datasets. The SMAP is a NASA Earth satellite launched on January 31, 2015, which combines active and passive microwaves to observe SM. To fulfil the demands of diverse applications, the SMAP dataset has four levels of products at spatial resolutions of 3 km, 9 km and 36 km (Mishra et al., 2017). Specifically, the SMAP level 4 Global 3-hourly 9 km EASE-Grid Surface and Root Zone Soil Moisture Analysis Update (SPL4SMAU) product, including both SSM and RZSM, at a spatial resolution of 9 km were used for further investigation. The SPL4SMAU provides estimates of global SSM and RZSM by assimilating the SMAP L-band brightness temperature data into NASA's Catchment land surface model (Reichle, 2017). In addition, disaggregated precipitation data were further used to correct the assimilated SSM and RZSM. It is noted that the SPL4SMAU product can provide continuous global SSM within 5 cm and RZSM at a depth of 100 cm. Several recent studies have highlighted the relatively high accuracy of the SPL4SMAU product (Nadeem et al., 2022). In the present study, a 0.05° SSM and RZSM dataset was initially obtained by resampling the original SPL4SMAU SSM product and SPL4SMAU RZSM product, and subsequently used to assess the estimated daily/ 0.05° SSM and RZSM over the study area. The SPL4SMAU product was acquired from the SMAP website (<https://nsidc.org/data/smap/data>).

3.2.4. CLDAS products

In addition to the SMAP products, the China Meteorological Administration Land Data Assimilation System (CLDAS) SSM and RZSM products were also used to evaluate the estimated SSM and RZSM. In the present study, the daily SSM and RZSM of the latest CLDAS version 2.0 (CLDAS-v2.0) with a spatial resolution of 0.0625° were initially resampled to 0.05° for further evaluation of the derived SSM and RZSM. The primary rationale for the selection of the CLDAS products is that CLDAS generally outperforms other available assimilated datasets over the China region, not only in terms of higher spatiotemporal resolution but also with better data quality as it assimilates observations from approximately 2400 quality-controlled national automatic stations and

nearly 40,000 regional automatic weather stations in China (Shi et al., 2011). Specifically, extensive assessments of the CLDAS SSM and RZSM products have indicated significant agreements with in-situ measurements in the previous literature (Liu et al., 2021a; Liu et al., 2021b; Wang and Li, 2020). The CLDAS product was obtained from the China Meteorological Data Service Centre (<https://data.cma.cn/en>).

4. Results

4.1. Optimized SMAR parameters over the study area

The SMAR parameters ($S_{c,surf}$, $S_{w,root}$, α , β) were optimized pixel-to-pixel over the study region using the MCMC algorithm described in Section 2.2. Fig. 3 depicts the spatial distribution of the four SMAR parameters ($S_{c,surf}$, $S_{w,root}$, α , β) at a 0.05° spatial resolution. $S_{c,surf}$ tends to be higher in southern and northeastern China, and $S_{c,surf}$ tends to be lower in parts of the northeast, which is close to the North China Plain and southwest China. The value is reasonably consistent and evenly distributed in most areas. The distributions of $S_{w,root}$ and $S_{c,surf}$ are particularly comparable, except for the northwest Xinjiang area, which has a minimal $S_{w,root}$ value.

To further analyze the characteristics of the four parameters, the histogram of the frequency distribution of the four parameters over the study area is plotted and shown in Fig. 4. Based on the results, it is evident that $S_{c,surf}$ generally follows a regular normal distribution with a mean value of 0.391 and a standard variance of 0.137. A similar pattern can also be observed for $S_{w,root}$, with the mean value and standard variance being 0.371 and 0.160, respectively. Moreover, both $S_{c,surf}$ and $S_{w,root}$ are typically spread in the range of 0.2–0.6, with a small percentage of pixels (approximately a percentage of 3.3 % and 4.9 %) having lower values below 0.1 or higher values over 0.7. In general, the pixels with lower $S_{w,root}$ values are mainly found in the desert regions of northwest China (e.g., Taklimakan desert shown in Fig. 3). As for α and β , a similar but significantly skewed distribution can be observed for these two parameters across the study area. In general, both α and β are typically spread in the range of 0.0–0.4, with only a small percentage of pixels (approximately, 0.7 % for α and 6.3 % for β) having higher values above 0.4.

Except for the spatial distribution characteristics of the four optimized parameters, understanding the accuracy of the SMAR model is essential for RZSM estimation. Fig. 5 illustrates the accuracy of the SMAR model for each pixel during the calibration stage based on the two commonly used criteria of RMSE and R . It is evident that most areas in northern China exhibit relatively high accuracy, with RMSE below $0.02 \text{ cm}^3/\text{cm}^3$. However, in some parts of the south, RMSE generally varies between $0.02 \text{ cm}^3/\text{cm}^3$ and $0.04 \text{ cm}^3/\text{cm}^3$, and only a few pixels may exhibit RMSE between $0.04 \text{ cm}^3/\text{cm}^3$ and $0.06 \text{ cm}^3/\text{cm}^3$. It is also worth noting that a small number of pixels have larger RMSE exceeding $0.06 \text{ cm}^3/\text{cm}^3$, which can be generally attributed to the uncertainties of the ERA5-Land data in these areas. Additionally, it is observed that the majority of the pixels demonstrate a significant correlation of over 0.8.

By regulating water infiltration, evaporation, and other water cycle processes, it is widely acknowledged that vegetation, soil properties and topography are key factors that influence the spatiotemporal dynamics of soil moisture under different climate conditions (Western et al., 2004). It is also noted that the ERA5-Land inherits the framework of model physics, data assimilation and core dynamics from the previous version and combines vast amounts of historical observations into global estimates using advanced modeling and data assimilation systems, where vegetation, soil properties and topography should be provided as essential inputs (Albergel et al., 2018). Hence, the ERA5-Land datasets (SSM, RZSM, runoff and total evaporation) used for the optimization of the SMAR parameters, can represent the variabilities for each grid with a unique combination of vegetation, soil properties, topography and climate conditions. Regarding the optimization of the SMAR model with the ERA-5 Land reanalysis, the finally optimized pixel-to-pixel SMAR

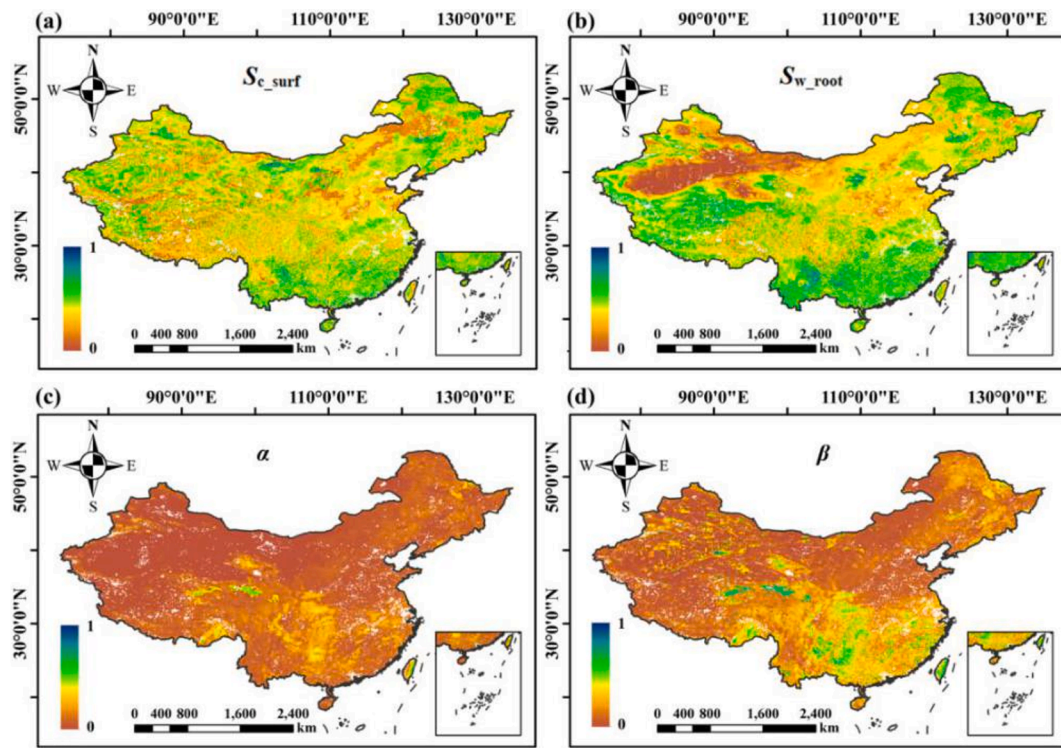


Fig. 3. Distribution of SMAR parameters (S_{c_surf} , S_{w_root} , α , β) at a spatial resolution of 0.05° over the study area. (a) Relative field capacity at the first layer (S_{c_surf}), (b) relative wilting level at the second layer (S_{w_root}), (c) water loss coefficient (α), (d) diffusion coefficient (β).

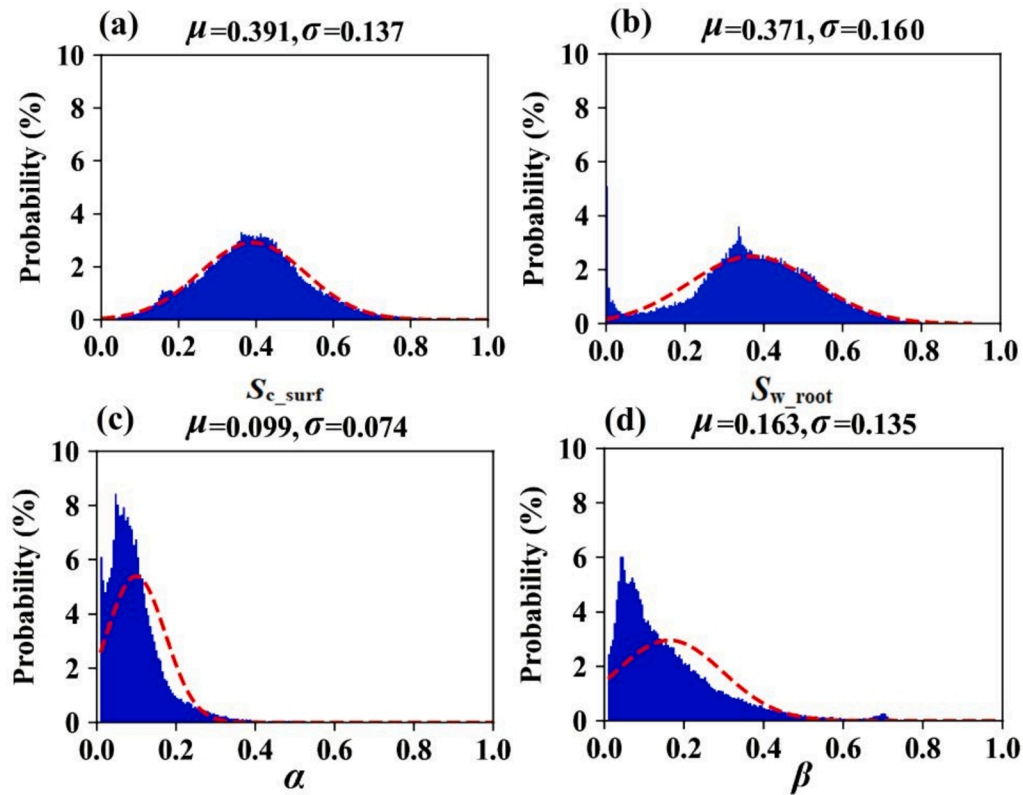


Fig. 4. The histogram of the frequency distribution of the four optimized parameters (S_{c_surf} , S_{w_root} , α , β). (a) Relative field capacity at the first layer (S_{c_surf}), (b) relative wilting level at the second layer (S_{w_root}), (c) water loss coefficient (α), (d) diffusion coefficient (β).

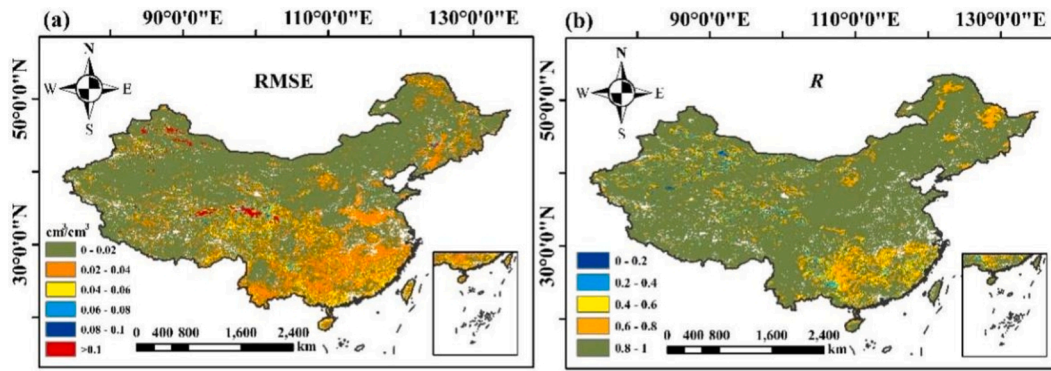


Fig. 5. RMSE (R) between actual RZSM and estimated RZSM during the optimization process.

parameters (S_{c_surf} , S_{w_root} , α , β) in Fig. 3 and corresponding accuracies in Fig. 5 can also reflect their spatial variabilities across grids with different underlying surface and climate conditions. Consequently, these variabilities of optimized SMAR parameters would directly affect RZSM estimates with the proposed approach.

Fig. 6 further illustrates the statistics of RMSE and R over the study region. The percentages of pixels with RMSE under $0.02 \text{ cm}^3/\text{cm}^3$ and between $0.02 \text{ cm}^3/\text{cm}^3$ and $0.04 \text{ cm}^3/\text{cm}^3$ can reach approximately 70 % and over 20 %, respectively. This indicates that over 90 % of the pixels have relatively high accuracy (e.g., RMSE below $0.04 \text{ cm}^3/\text{cm}^3$) for RZSM estimation. Regarding R , it is clear that nearly 85 % of the entire pixels reveal a significant correlation between the estimated RZSM and actual values with R over 0.8. All these results indicate significant accuracy of the SMAR optimization, which can guarantee the retrieval accuracy of RZSM to a certain extent.

4.2. Assessment of SSM

To obtain RZSM using the SMAR model, it is crucial to evaluate the satellite-derived SSM data before applying them to the study area. Based on the method in the previous section, a daily/ 0.05° SSM was first obtained from the synergetic use of satellite observations and reanalysis data following the method proposed by Fang et al. (2022). Taking four typical days (January 15th for winter, April 15th for spring, July 15th for summer and October 15th for autumn) in 2019 as an example, Fig. 7

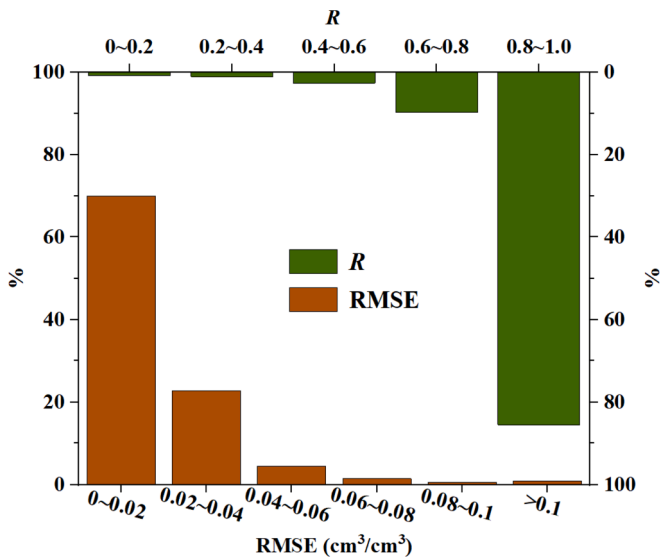


Fig. 6. Percentages of RMSE and R at different levels for actual RZSM and estimated RZSM during the optimization process. The left and lower axes represent RMSE, and the right and upper axes represent R .

depicts the spatial distribution of the estimated SSM at a spatial resolution of 0.05° .

Due to the absence of ground SSM truth at a spatial resolution of 0.05° , two referenced SSM products, namely the SPL4SMAU and CLDAS, were used to preliminarily evaluate the estimated SSM. Specifically, the SPL4SMAU SSM and CLDAS products were resampled from $\sim 0.09^\circ$ to 0.05° and from 0.0625° to 0.05° using nearest neighbor interpolation, respectively. Fig. 8 illustrates 1000 random sample pixels generated using the equidistant random sampling method across mainland China (Leng et al., 2019). Figure 9 and Fig. 10 show the scatterplots between the estimated SSM and the resampled SPL4SMAU SSM, and between the estimated SSM and the resampled CLDAS SSM on the four selected days in 2019, respectively. According to the results presented in Figure 9, the scatterplots are uniformly distributed on both sides of the 1:1 line, with significant R values ranging from 0.714 to 0.795, indicating a relatively high correlation between the estimated SSM and the SMAP SSM product. Moreover, the RMSE generally ranges from $0.074 \text{ cm}^3/\text{cm}^3$ to $0.086 \text{ cm}^3/\text{cm}^3$ with biases ranging from $0.015 \text{ cm}^3/\text{cm}^3$ to $0.048 \text{ cm}^3/\text{cm}^3$, revealing that the SSM is often overestimated when compared to the SPL4SMAU SSM. Based on the RMSE and bias, the ubRMSE generally fluctuates between $0.062 \text{ cm}^3/\text{cm}^3$ and $0.076 \text{ cm}^3/\text{cm}^3$. Specifically, the overall statistical criteria of RMSE, bias, ubRMSE and R are $0.080 \text{ cm}^3/\text{cm}^3$, $0.037 \text{ cm}^3/\text{cm}^3$, $0.070 \text{ cm}^3/\text{cm}^3$ and 0.742, respectively. These statistical values are comparable to those of previous studies (Fang et al., 2022; Ranney et al., 2015; Senanayake et al., 2019). As for the comparison between the estimated SSM and the CLDAS SSM product, similar results were found in the four selected days. The RMSE (bias) varies from $0.064 \text{ cm}^3/\text{cm}^3$ ($-0.013 \text{ cm}^3/\text{cm}^3$) to $0.080 \text{ cm}^3/\text{cm}^3$ ($0.045 \text{ cm}^3/\text{cm}^3$), which results in fair ubRMSE between $0.064 \text{ cm}^3/\text{cm}^3$ to $0.076 \text{ cm}^3/\text{cm}^3$. In addition, considerable R ranging from 0.694 to 0.805 was obtained between the two SSM datasets. The overall statistical criteria of RMSE, bias, ubRMSE and R are $0.074 \text{ cm}^3/\text{cm}^3$, $0.009 \text{ cm}^3/\text{cm}^3$, $0.070 \text{ cm}^3/\text{cm}^3$ and 0.743, respectively. All these results confirmed that the estimated SSM can be reasonably used as the essential input for estimating RZSM with the proposed approach.

4.3. Assessment of RZSM

Based on the estimated daily/ 0.05° SSM and optimized SMAR parameters, the daily/ 0.05° RZSM dataset over the study region was obtained using the proposed method. Similar to the previous section, Fig. 11 illustrates the spatial distribution of the estimated RZSM at a spatial resolution of 0.05° on the four typical days in 2019. The results show that the RZSM is notably high in the south of the Yangtze River, followed by northeastern China and the Tibetan Plateau in the west. Moreover, RZSM is quite low in the desert regions in Xinjiang and Inner Mongolia. Overall, the RZSM content drops gradually from south to north and from east to west in mainland China.

Similar to the evaluations of SSM in the previous section, the

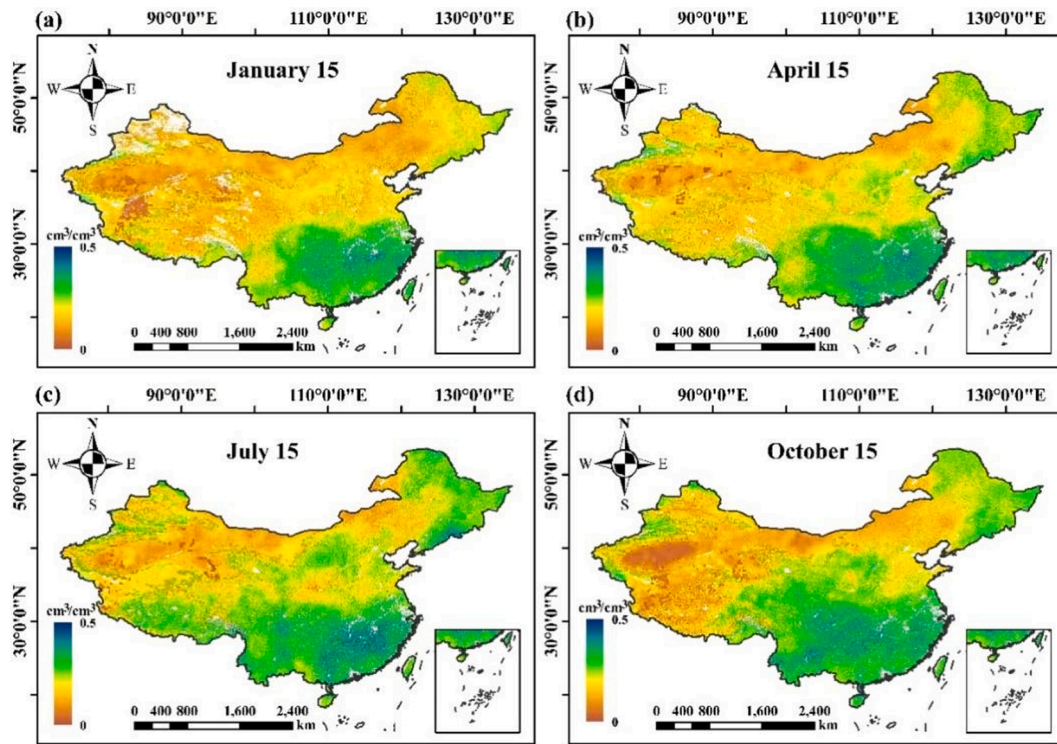


Fig. 7. Estimated daily/0.05° SSM over the study area on January 15th, April 15th, July 15th and October 15th in 2019.

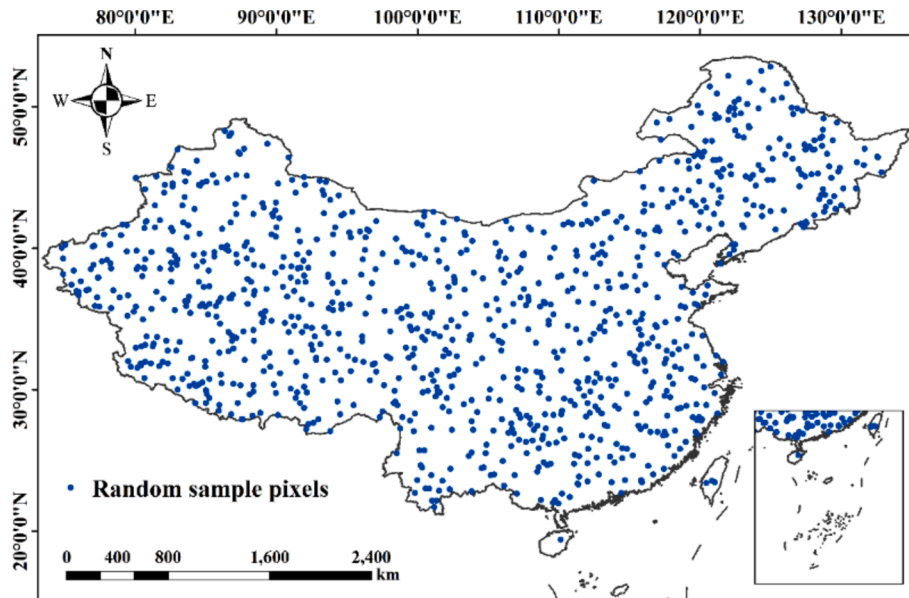


Fig. 8. Spatial distribution of 1000 sample pixels over the study region.

SPL4SMAU RZSM and CLDAS RZSM products were resampled to 0.05° to assess the estimated RZSM due to the lack of in-situ RZSM measurements at that spatial resolution. The comparisons between the estimated RZSM and the SPL4SMAU RZSM on the four typical days in 2019 are shown in Fig. 12. Specifically, the same random sample pixels used for assessing satellite-derived SSM in the previous section were used to evaluate the estimated RZSM in the present section. The results indicate that scatterplots are evenly dispersed along the 1:1 line with RMSE and bias varying from 0.091 cm³/cm³ to 0.097 m³/cm³ and 0.043 cm³/cm³ to 0.060 cm³/cm³, respectively. In addition, a fair correlation of 0.557 to 0.655 can be observed on the four selected days. Following the statistics,

the ubRMSE of the estimated RZSM varied from 0.075 cm³/cm³ to 0.084 cm³/cm³. Specifically, the overall statistical criteria of RMSE, bias, ubRMSE and R are 0.095 cm³/cm³, 0.050 cm³/cm³, 0.080 cm³/cm³ and 0.611, respectively. Fig. 13 shows the comparison between the estimated RZSM and CLDAS RZSM products on the selected days. Following the results, the correlation coefficient between the two RZSM datasets varies from 0.496 to 0.596, and the RMSE (bias) generally fluctuates from 0.083 cm³/cm³ (−0.030 cm³/cm³) to 0.110 cm³/cm³ (0.058 cm³/cm³). Based on these results, fair ubRMSE between 0.080 cm³/cm³ to 0.097 cm³/cm³ was obtained between the two RZSM datasets. Specifically, the overall statistical criteria of RMSE, bias,

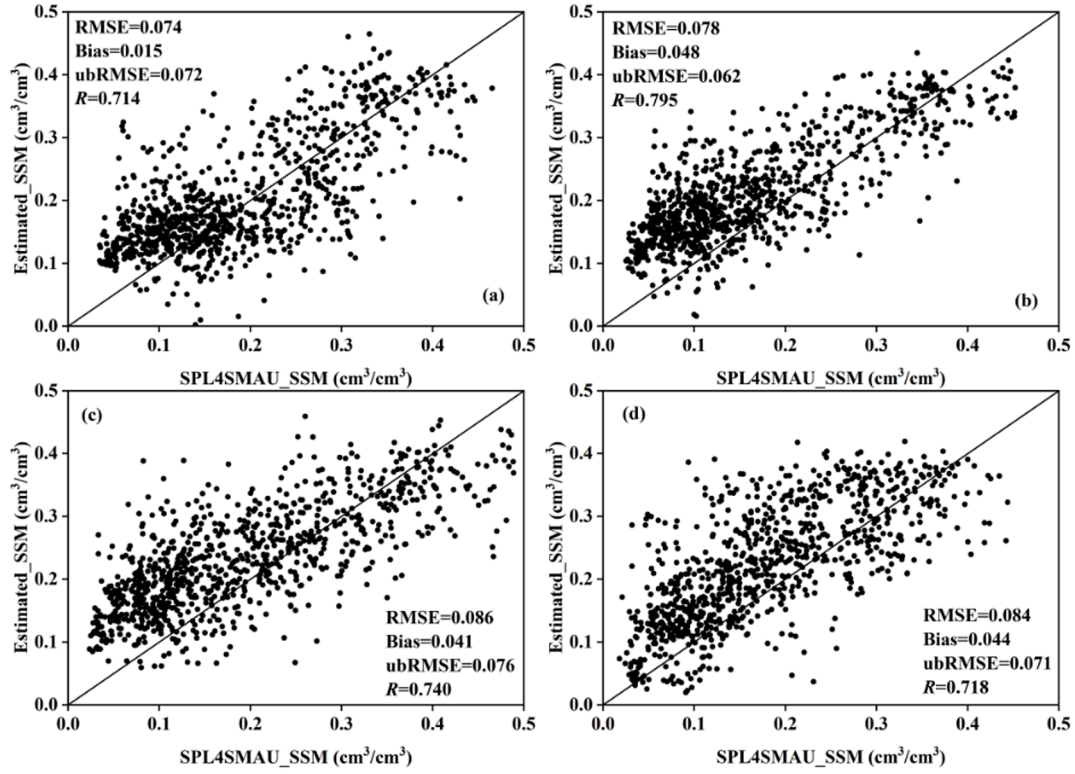


Fig. 9. Comparison between estimated SSM and the SPL4SMAU SSM product at 0.05° in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

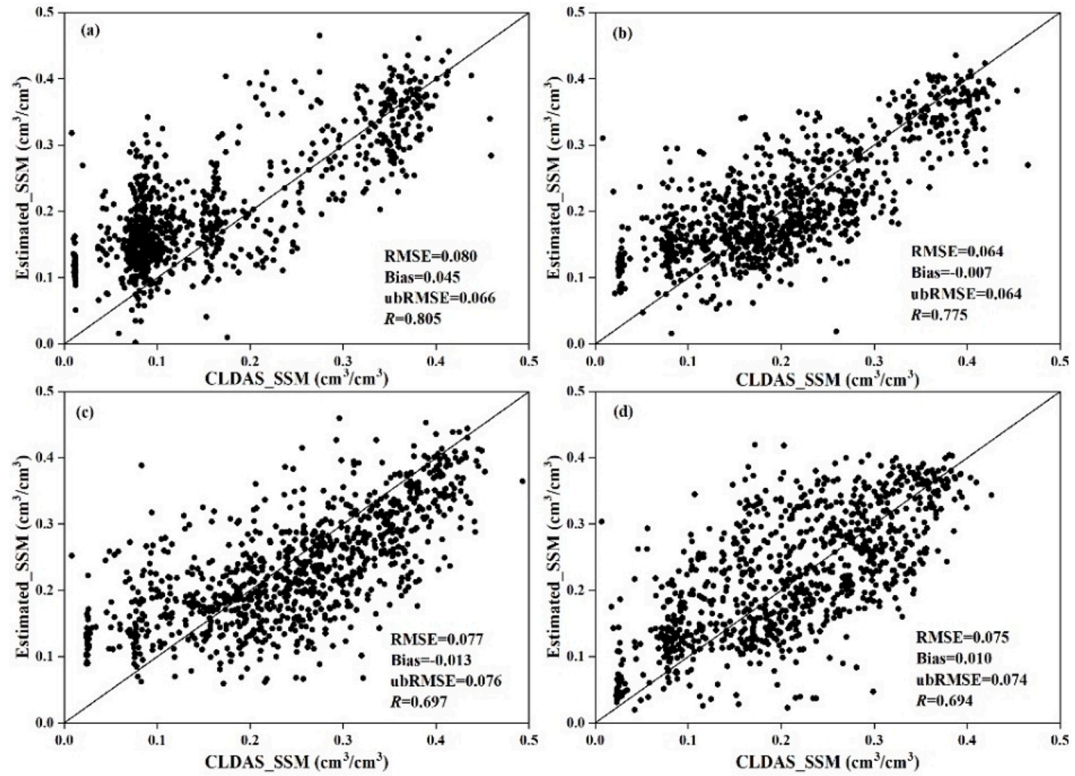


Fig. 10. Comparison between estimated SSM and the CLDAS SSM product at 0.05° in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

ubRMSE and R are $0.094 \text{ cm}^3/\text{cm}^3$, $0.004 \text{ cm}^3/\text{cm}^3$, $0.088 \text{ cm}^3/\text{cm}^3$ and 0.542 , respectively. All these results indicate an acceptable accuracy of RZSM estimation over the study area.

4.4. Retrieval accuracy of RZSM over different land cover types

To further investigate the accuracy of the estimated RZSM over different land cover types, we selected 1000 random pixels for each land

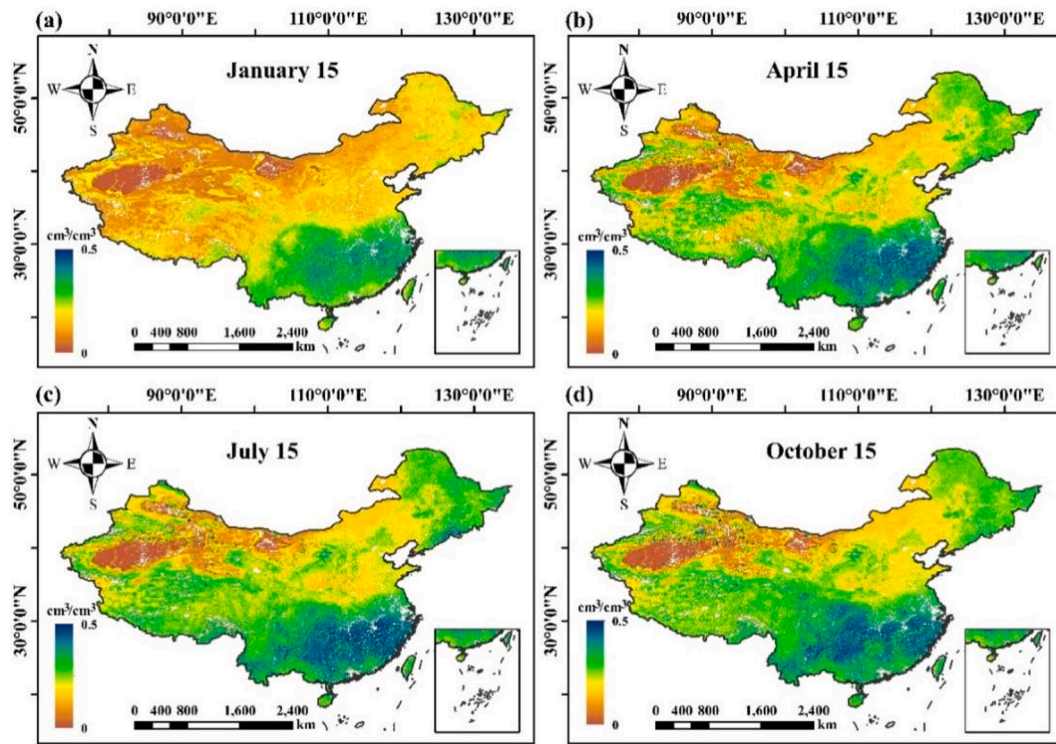


Fig. 11. Estimated daily/0.05° RZSM over the study area on January 15th, April 15th, July 15th and October 15th in 2019.

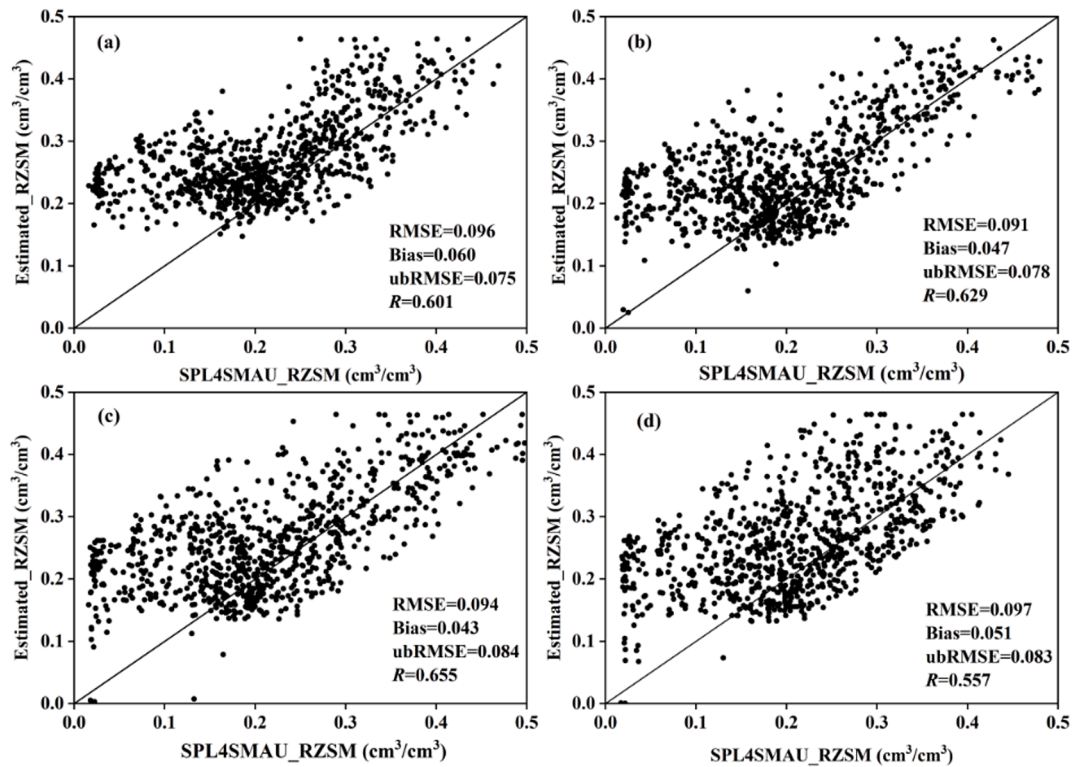


Fig. 12. Comparison between estimated RZSM and the SPL4SMAU RZSM product at 0.05° in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

cover type of croplands, grasslands, and woodlands. Fig. 14 depicts the samples for each land cover type based on the MCD12Q1C product over the study region. The following subsections illustrate the retrieval accuracy of RZSM compared to the SPL4SMAU RZSM and CLDAS RZSM products at 0.05° over different land cover types.

4.4.1. Croplands

Understanding the dynamics of RZSM over croplands is crucial for China, which is one of the largest farming countries where RZSM plays a significant role in crop growth. As shown in Fig. 14, the cropland sample pixels are mostly distributed in the Northeast Plain, North China Plain,

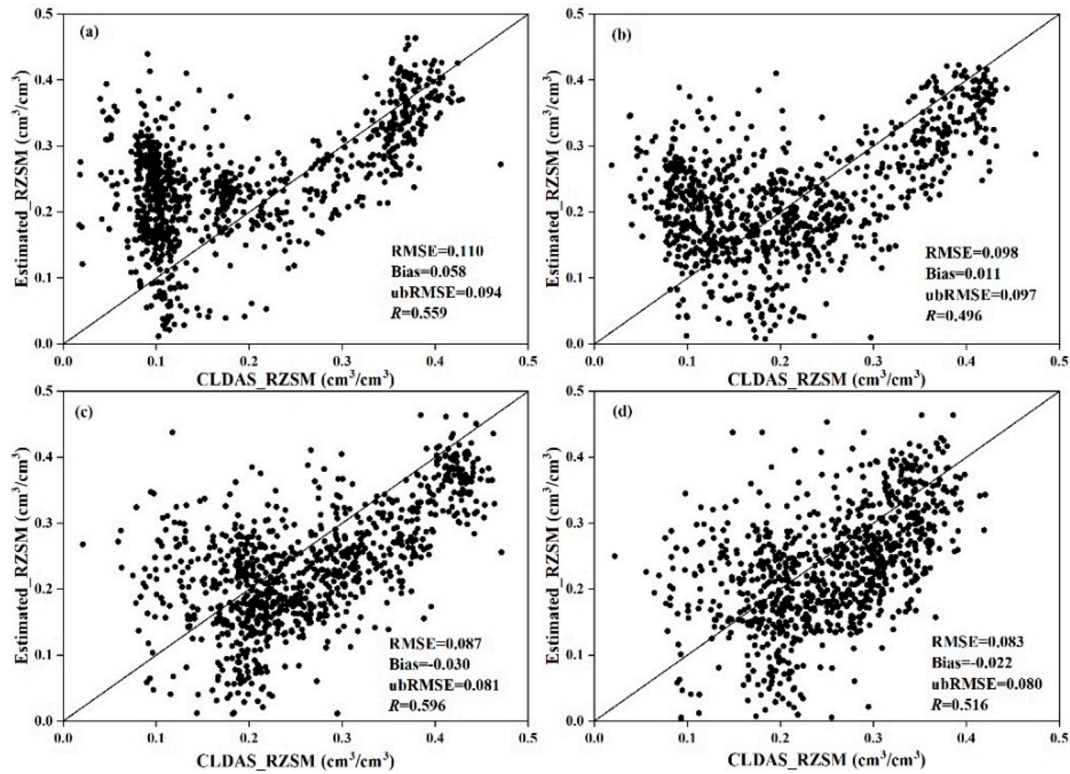


Fig. 13. Comparison between estimated RZSM and the CLDAS_RZSM product at 0.05° in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

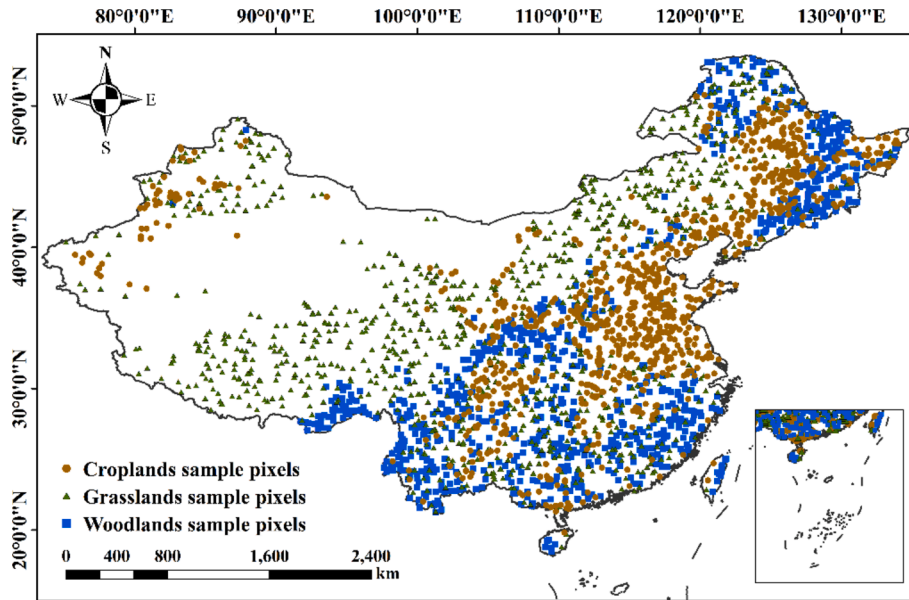


Fig. 14. Distribution of 3000 sample pixels in croplands, grasslands and woodlands.

Middle-Lower Yangtze Plain and South China. Fig. 15 shows the scatterplots between the estimated RZSM and SPL4SMAU RZSM for the cropland sample pixels on the four selected days in 2019. The two RZSM were evenly distributed around the 1:1 line, with RMSE varying from 0.060 cm³/cm³ to 0.074 cm³/cm³ for the selected four days. Moreover, a slight bias from 0.002 cm³/cm³ to 0.024 cm³/cm³ and an acceptable *R* from 0.472 to 0.708 can be observed between the two RZSM datasets. Based on these results, the ubRMSE during the study period generally fluctuates between 0.055 cm³/cm³ and 0.073 cm³/cm³. Meanwhile, the assessment of estimated RZSM using CLDAS RZSM in Fig. 16 indicated a

relatively high accuracy with RMSEs ranging from 0.060 cm³/cm³ to 0.073 cm³/cm³ and *R* ranging from 0.588 to 0.785. However, there was an underestimation of the estimated RZSM when compared to CLDAS RZSM, with a bias ranging from 0.046 cm³/cm³ to -0.017 cm³/cm³. Nevertheless, the ubRMSE of the two RZSM datasets varies in the range of 0.053 cm³/cm³ and 0.064 cm³/cm³, indicating significantly accurate estimations for RZSM over croplands.

4.4.2. Grasslands

After croplands, grasslands are the second dominant land cover type

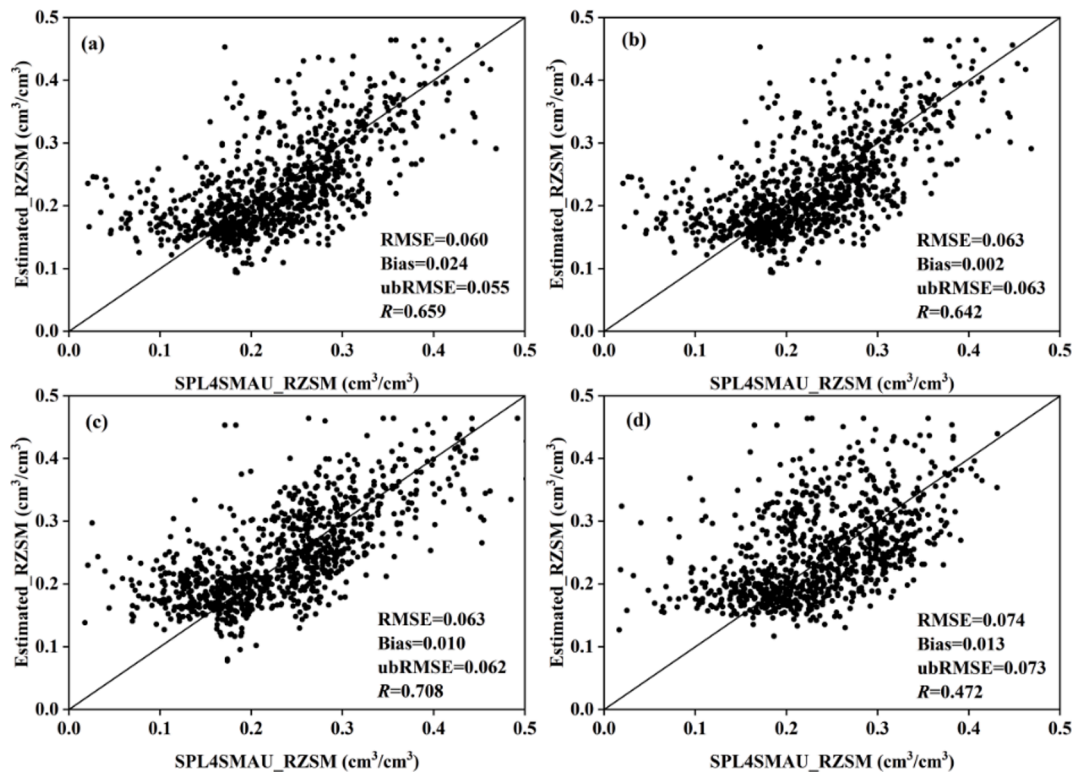


Fig. 15. Comparison between estimated 0.05° RZSM and the SPL4SMAU RZSM product over croplands in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

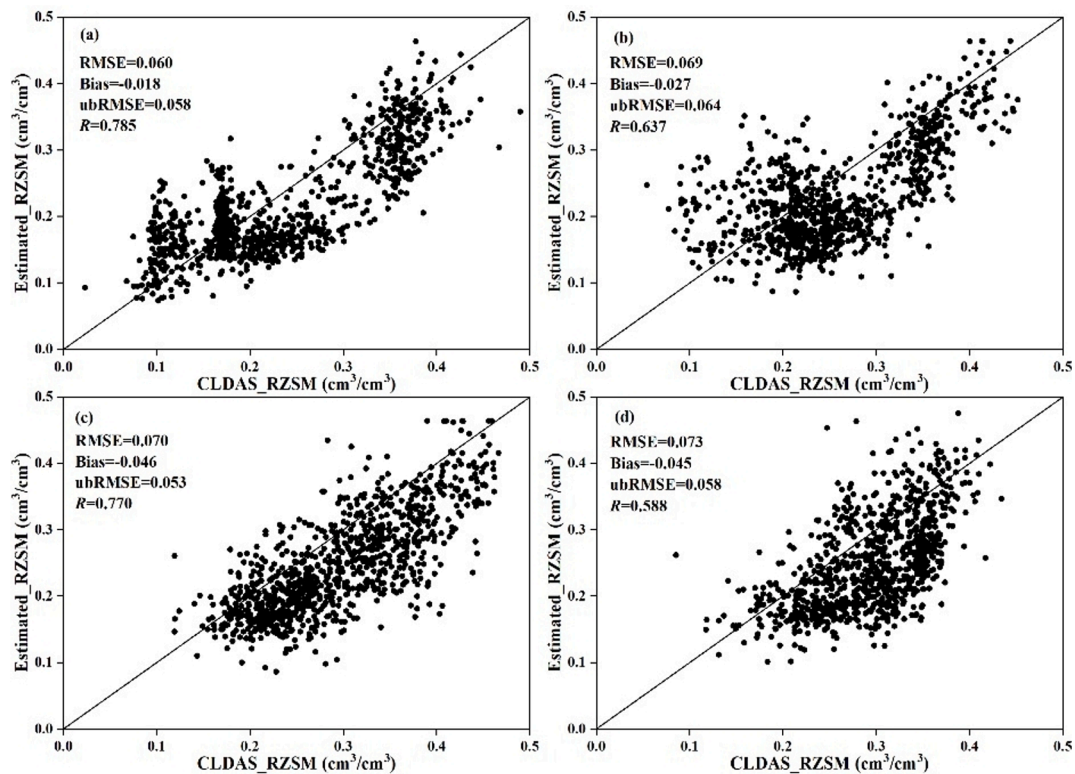


Fig. 16. Comparison between estimated 0.05° RZSM and the CLDAS RZSM product over croplands in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

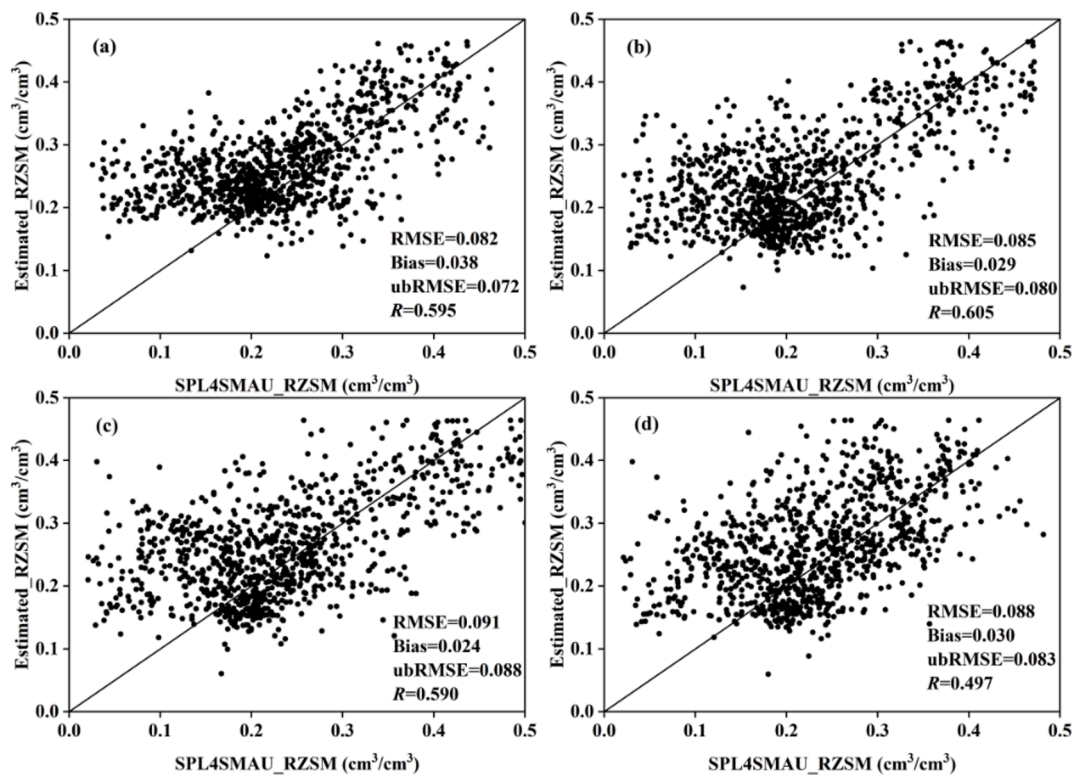


Fig. 17. Comparison between estimated 0.05° RZSM and the SPL4SMAU RZSM product over grasslands in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

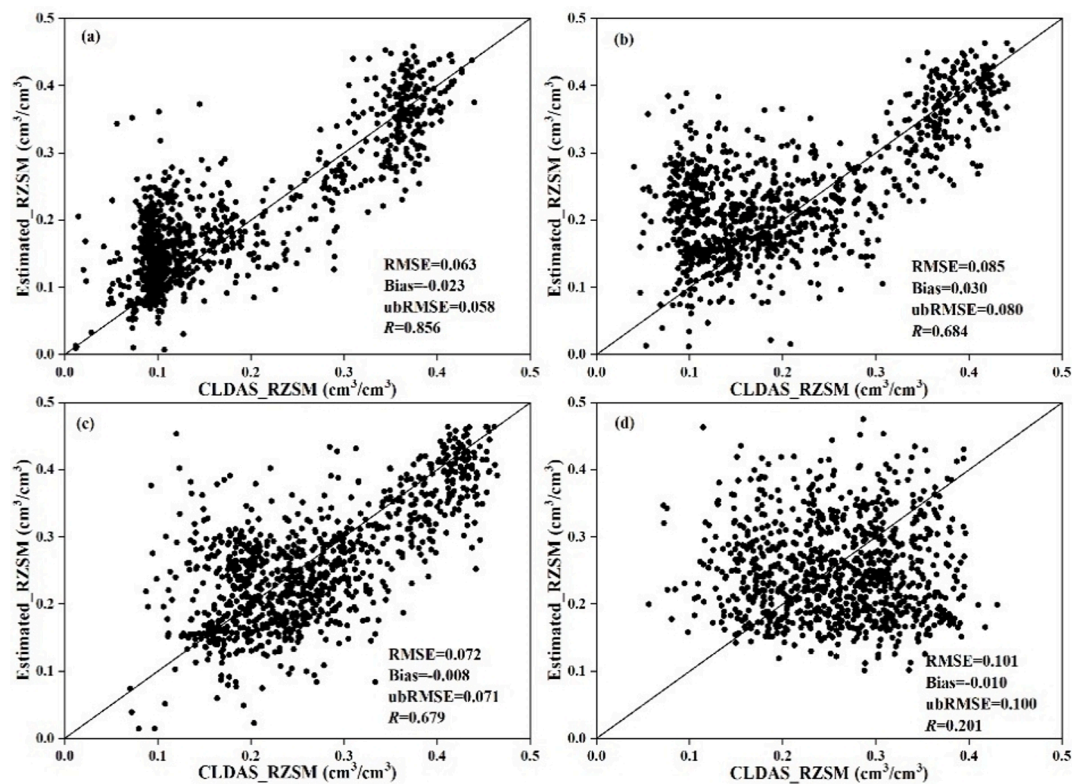


Fig. 18. Comparison between estimated 0.05° RZSM and the CLDAS RZSM product over grasslands in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

in China and play an essential role in agricultural ecosystems. As shown in Fig. 12, the grassland sample pixels are mostly distributed in the eastern part of Inner Mongolia, southwestern China and the northern part of Xinjiang Province. Fig. 17 shows the scatterplots between the estimated RZSM and SPL4SMAU RZSM for the grassland sample pixels on the four selected days in 2019. The results indicate a slightly decreased accuracy in both RMSE and bias compared to those over the croplands. For the four selected days, RMSE generally varies from 0.082 cm^3/cm^3 to 0.091 cm^3/cm^3 , whereas bias fluctuates from 0.024 cm^3/cm^3 to 0.038 cm^3/cm^3 . On these bases, a fair ubRMSE from 0.072 cm^3/cm^3 to 0.088 cm^3/cm^3 can be obtained from the statistics. Except for these, the correlation coefficient between the two RZSM datasets is found to vary between 0.497 and 0.605. As for the comparison with CLDAS RZSM shown in Fig. 18, a similar slightly decreased accuracy was found when compared to the accuracy over the croplands. Specifically, the RMSEs on the four selected days vary from 0.063 cm^3/cm^3 to 0.101 cm^3/cm^3 , whereas bias fluctuates in a range of $-0.023 \text{ cm}^3/\text{cm}^3$ to 0.030 cm^3/cm^3 . In addition, except for the assessment on October 15th, the two datasets are well correlated with R ranging from 0.679 to 0.856. Nevertheless, the averaged ubRMSE of the two RZSM datasets is approximately 0.077 cm^3/cm^3 . All these results confirm that the proposed approach generally reveals worse performance over grasslands than croplands. However, the accuracy of the estimated RZSM over grassland is still acceptable considering the criterion of ubRMSE.

4.4.3. Woodlands

Woodlands play a crucial role in regulating temperature and climate at local to regional scales, which is essential for preserving biodiversity and conserving water. As shown in Fig. 12, the woodland sample pixels are mostly distributed in the Northeast Plain and South China. Fig. 19 illustrates the scatterplots between the estimated RZSM and SPL4SMAU RZSM in woodlands on the four selected days in 2019. The figure indicates that the RMSE and bias generally varied within a range of 0.066–0.078 cm^3/cm^3 and 0.013–0.038 cm^3/cm^3 , respectively.

Moreover, the ubRMSE also falls between those of the aforementioned land cover types with a value between 0.064 cm^3/cm^3 and 0.077 cm^3/cm^3 . In addition, the correlation coefficient between the two RZSM datasets is also in a reasonable range of 0.314–0.667. Furthermore, following the results presented in Fig. 20, the RMSE and bias generally varied within a range of 0.062–0.083 cm^3/cm^3 and -0.020 – $0.027 \text{ cm}^3/\text{cm}^3$, respectively. In addition, the two datasets also exhibit a fair correlation with R varying from 0.420 to 0.827. These statistics indicated that ubRMSE of 0.059–0.078 cm^3/cm^3 can be obtained, suggesting an intermediate level of accuracy when compared to croplands and grassland. Overall, these results demonstrate that the proposed approach can obtain fair RZSM over woodlands.

4.4.4. Comparisons of RZSM estimation over different land cover types

To comprehensively assess the accuracy of RZSM estimations for different land cover types, the estimated RZSM for each land cover type on the four selected days was combined to evaluate the overall performance in this section. Table 3 and Table 4 summarize the overall statistical criterion between the estimated RZSM and SPL4SMAU RZSM, and between the estimated RZSM and CLDAS RZSM, respectively, for the three dominant land cover types. Overall, for the assessment with SPL4SMAU RZSM (CLDAS RZSM) the RMSEs between the two RZSM datasets are 0.065 cm^3/cm^3 (0.069 cm^3/cm^3), 0.087 cm^3/cm^3 (0.081 cm^3/cm^3) and 0.072 cm^3/cm^3 (0.069 cm^3/cm^3) for croplands, grasslands and woodlands, respectively. The overall biases for these three land cover types are 0.012 cm^3/cm^3 ($-0.035 \text{ cm}^3/\text{cm}^3$), 0.030 cm^3/cm^3 (0.010 cm^3/cm^3) and 0.014 cm^3/cm^3 (0.006 cm^3/cm^3), respectively. Both the RMSE and bias result in ubRMSE values of 0.064 cm^3/cm^3 (0.059 cm^3/cm^3), 0.081 cm^3/cm^3 (0.080 cm^3/cm^3) and 0.071 cm^3/cm^3 (0.069 cm^3/cm^3) for croplands, grasslands and woodlands, respectively. Furthermore, the significant R values between the two datasets for the three land cover types are 0.621 (0.711), 0.573 (0.660) and 0.581 (0.700). All these results confirm the reasonable accuracy of the proposed approach for deriving RZSM.

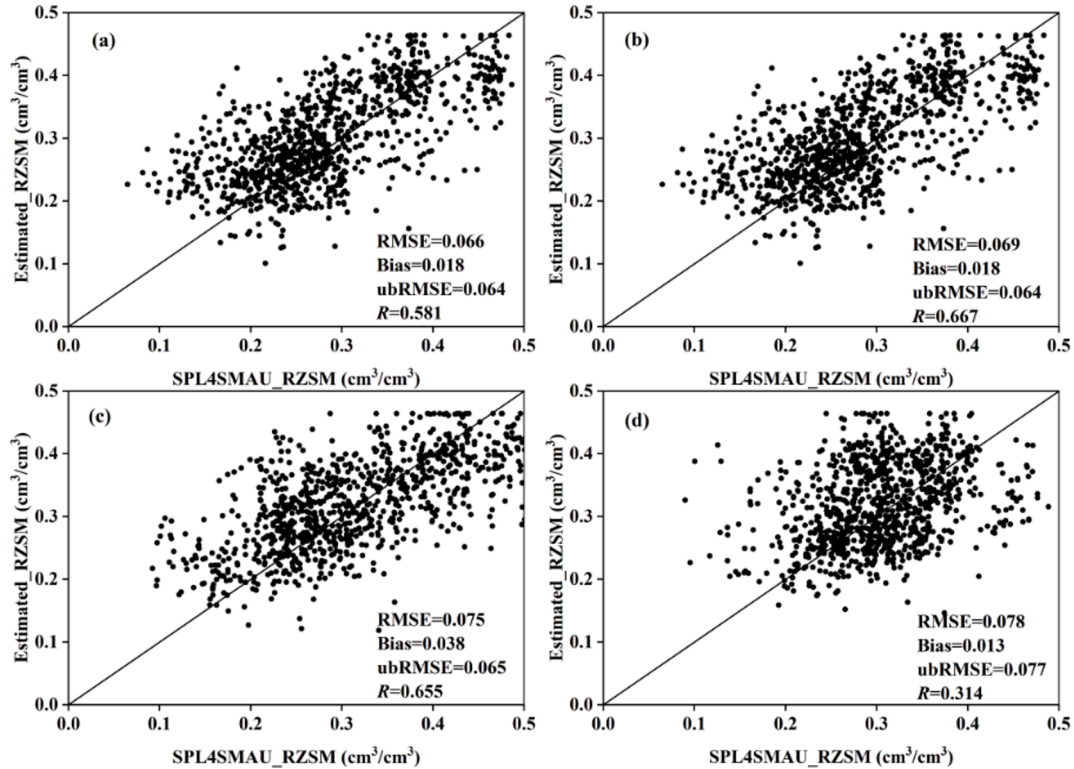


Fig. 19. Comparison between the estimated 0.05° RZSM and the SPL4SMAU RZSM product over woodlands in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

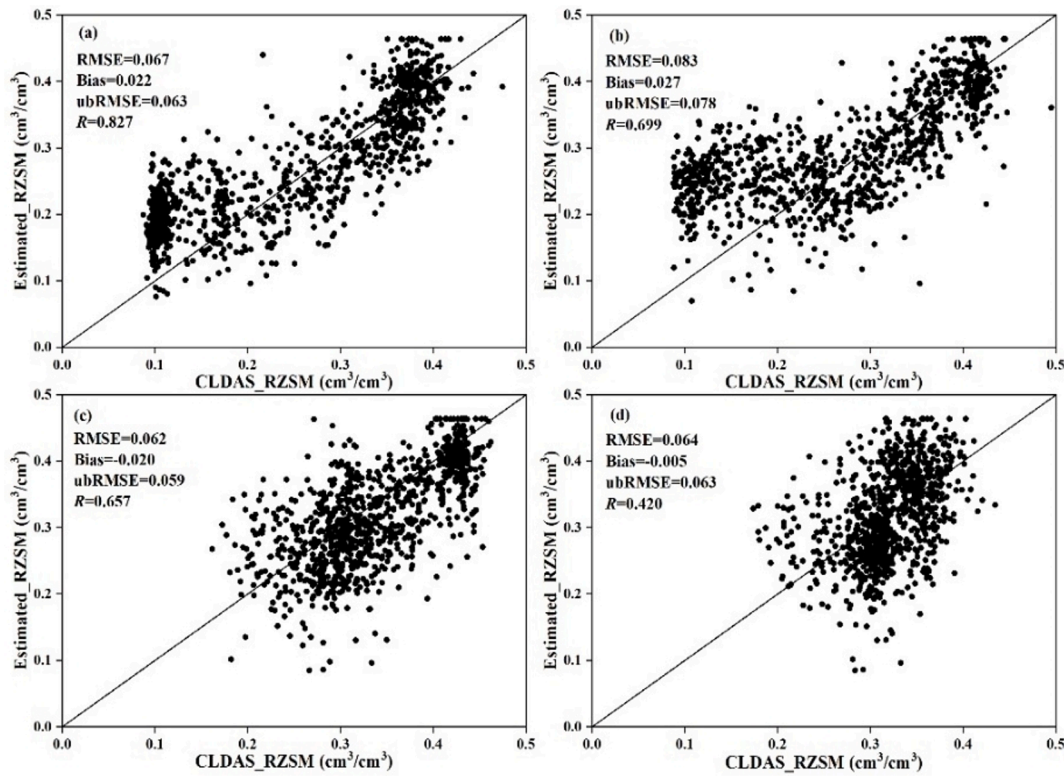


Fig. 20. Comparison between the estimated 0.05° RZSM and the CLDAS RZSM product over woodlands in 2019. (a) January 15th, (b) April 15th, (c) July 15th, (d) October 15th.

Table 3

The overall error statistics when assessed with SPL4SMAU RZSM product.

	RMSE (cm ³ /cm ³)	Bias (cm ³ /cm ³)	ubRMSE (cm ³ /cm ³)	R
Croplands	0.065	0.012	0.064	0.621
Grasslands	0.087	0.030	0.081	0.573
Woodlands	0.072	0.014	0.071	0.581

Table 4

The overall error statistics when assessed with CLDAS RZSM product.

	RMSE (cm ³ /cm ³)	Bias (cm ³ /cm ³)	ubRMSE (cm ³ /cm ³)	R
Croplands	0.069	-0.035	0.059	0.711
Grasslands	0.081	0.010	0.080	0.660
Woodlands	0.069	0.006	0.069	0.700

However, the performance of the proposed approach may vary across land cover types. This is generally reasonable because satellite-derived SSM exhibits various accuracies over different landscapes (Guo et al., 2020; Wang et al., 2010; Zucco et al., 2014). Moreover, different vegetation systems are also characterized by different soil structures, which can affect RZSM estimation with the proposed method.

5. Discussion

5.1. Effects of SSM uncertainties on RZSM estimation

The current study has established a practical framework for generating daily/0.05° RZSM by integrating the SMAR model and satellite-derived SSM estimates. Specifically, the SMAR model parameters can be optimized pixel-to-pixel using Bayesian inference implemented by the MCMC algorithm, with the ERA5-Land data provided as inputs. A

preliminary assessment of the estimated RZSM reveals an overall overestimation when compared to the SPL4SMAU product, which can most likely be attributed to the overestimation of the satellite-derived SSM, as shown in Figure 9, where an overall bias of 0.037 cm³/cm³ can be found between the two SSM datasets. Hence, it is of great interest to further investigate the SMAR performance with the corrected SSM. To this end, we primarily corrected the estimated SSM with the bias for each day and further set it as input for the same day for estimating RZSM. Similar to Sections 4.2 and 4.3, the estimated RZSM for the same 1000 random pixels was taken as an example to investigate the effects of the overestimation of the satellite-derived SSM on the RZSM prediction. Table 5 presents the error statistics of RMSE, bias, ubRMSE and R for the four selected days in 2019 with bias correction of the satellite-derived SSM dataset. Overall, the RMSE between the two datasets is 0.092 cm³/cm³ with a bias of 0.046 cm³/cm³, resulting in an ubRMSE of 0.080 cm³/cm³. In addition, the correlation coefficient of the two RZSM datasets is 0.607. These statistical criteria are generally comparable to the RZSM assessments with the original SSM presented in Section 4.3. However, the bias has been significantly decreased, indicating that it is essential to obtain reliable SSM estimates for predicting RZSM with the proposed method.

Table 5

Error statistics between estimated RZSM and SPL4SMAU RZSM with bias correction.

	RMSE (cm ³ /cm ³)	Bias (cm ³ /cm ³)	ubRMSE (cm ³ /cm ³)	R
Jan 15	0.092	0.056	0.073	0.617
Apr 15	0.089	0.043	0.078	0.612
Jul 15	0.093	0.039	0.084	0.650
Oct 15	0.094	0.046	0.082	0.547
Overall	0.092	0.046	0.080	0.607

5.2. Future developments

Although this study achieved acceptable accuracy in estimating RZSM compared to SPL4SMAU RZSM and CLDAS RZSM, there are still several limitations. First, the present study used the reanalysis datasets of ERA5-Land as the main input to optimize the four model parameters at 0.05° in the study area. It is evident that the accuracy of ERA5-Land would directly affect the optimized results, as well as the RZSM predictions. Although the results reveal a certain error with the SMAR optimization, it should be noted that ERA5-Land is most likely to be the most adequate dataset to obtain the SMAR parameters as well as RZSM at the national scale over a large region such as mainland China. Nevertheless, it is also an alternative to first collect sufficient synchronous ground measurements of SM profiles and meteorological records under different landscapes and climate patterns to optimize the SMAR model site-to-site and subsequently expand the site-based SMAR parameters to the regional scale. Future investigations can merge these two schemes to determine better SMAR parameters for applications.

In addition, the present study used the satellite-derived daily/ 0.05° SSM as an essential input for RZSM prediction. Although many SSM algorithms and products have been developed, it is understood that various uncertainties still exist in most of the currently available satellite SSM datasets. The accuracy of the SSM estimates plays a significant role in the determination of the RZSM with the proposed approach, which has also been confirmed in the previous section. The present study used SMOPS data to obtain spatially complete SSM data, as SMOPS shows a certain superiority to other satellite-based SSM products. Nevertheless, the SSM estimates still reveal a certain uncertainty with an overall ubRMSE of $0.070 \text{ cm}^3/\text{cm}^3$. While the SSM estimates are generally comparable to most of the current investigations, it is anticipated that more accurate SSM estimates can be generated to serve as input for the proposed approach in future developments. Moreover, because it is difficult to obtain RZSM pixel truth with in situ measurements at a spatial resolution of 0.05° in China, the present study has preliminarily assessed the estimated RZSM with the SPL4SMAU RZSM and CLDAS products. The accuracy of the preliminary assessments is more like a relative accuracy or a reference of the proposed RZSM over the study region, rather than the absolute accuracy. Moreover, the SMAP data have contributed to the production of both the SMOPS and SPL4SMAU RZSM, which may affect the independence in the accuracy assessments of the estimated RZSM. However, it is important to note that SMAP is just a small part of the determination of the SMOPS and the SPL4SMAU RZSM products. For the SMOPS product, SMAP and various other active and passive microwave data are combined to generate the SSM datasets (Wang et al., 2021). The SPL4SMAU RZSM product is produced from a complex land surface assimilation system that takes in a wide range of variables, including SMAP L-band brightness temperature, as inputs. Nevertheless, it is still expected that future in-depth validation of the estimated RZSM can be conducted in another study area where RZSM pixel truth can be obtained.

Finally, based on the SMAR model principle, the most significant water mass exchange between the surface and root layers is represented by infiltration. The assumption is that lateral water fluxes are negligible compared to infiltration, which is generally reasonable for flat areas that typically do not receive large amounts of lateral water drainage (Baldwin et al., 2017). However, it has been observed that lateral water fluxes can impact soil–water characteristics, especially in heterogeneous regions, leading to uncertainties in simulating SSM and RZSM (Rummler et al., 2022). Despite many studies demonstrating acceptable accuracies in estimating RZSM using the SMAR model without considering lateral water fluxes at a regional scale (Faridani et al., 2017; Baldwin et al., 2019; Farokhi et al., 2021), it is still anticipated that considering lateral water fluxes in the SMAR model has the potential to enhance RZSM prediction.

6. Conclusions

In the present study, a daily/ 0.05° RZSM dataset covering China was generated from the combined use of satellite-derived SSM estimates and the SMAR model. A crucial step for deriving the RZSM dataset is the optimization of the SMAR model. In this research, the MCMC algorithm was applied in the optimization process to obtain the pixel-to-pixel SMAR parameters using the ERA5-Land product. Due to the lack of in situ RZSM measurements and other ground SSM truth at a spatial resolution of 0.05° , the estimated RZSM dataset was preliminarily assessed with the resampled SPL4SMAU RZSM and CLDAS products at the same pixel size. The results indicated an overall acceptable accuracy with an ubRMSE of $\sim 0.07\text{--}0.090 \text{ cm}^3/\text{cm}^3$ over the study area. Further evaluation revealed various performances of the proposed approach over different land cover types. In summary, the present study provided a feasible framework for obtaining reliable RZSM estimates at the regional scale. Nevertheless, further study can focus on improving SSM estimates and optimizing the SMAR model at the regional scale to predict better RZSM.

CRediT authorship contribution statement

Yanyan Wang: Writing – original draft, Methodology, Investigation, Formal analysis, Data curation. **Pei Leng:** Writing – review & editing, Writing – original draft, Supervision, Software, Resources, Project administration, Methodology, Funding acquisition, Conceptualization. **Jianwei Ma:** Validation, Software, Data curation. **Salvatore Manfreda:** Supervision, Software. **Chunfeng Ma:** Writing – review & editing, Supervision, Data curation. **Qian Song:** Resources, Formal analysis. **Guo-Fei Shang:** Resources, Conceptualization. **Xia Zhang:** Software, Resources. **Zhao-Liang Li:** Writing – review & editing, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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